Week 4 Tuesday
L-7
Saha Part 2

$$A^r_{s_a} + \text{energy} \Longleftrightarrow A^{r+1}_{s_b} + e^-$$

Goal: find $\dfrac{n^r_A}{n_A}$

1a $$n^r = \frac{n^r_o}{g^r_o} U^r(T)$$

1b $$n^{r+1} = \frac{n^{r+1}_o}{g^{r+1}_o} U^{r+1}(T)$$

2a $$\frac{n^{r+1}_o}{n^r_o} n_e = \frac{g^{r+1}_o}{g^r_o} \frac{2(2\pi m_e kT)^{3/2}}{h^3} e^{-\chi_r/kT}$$

Unknowns:

n^r n^{r+1}

n^r_o n^{r+1}_o

n_e

$P_e = n_e kT$

In equation 3, substitute the ground state population for the total population with eps 1 and 2

$$\frac{n^{r+1}}{n^r} \boxed{P_e} = T^{5/2} e^{-\chi_r/kT} \frac{U^{r+1}(T)}{U^r(T)} \frac{2(2\pi m_e)^{3/2} k^{5/2}}{h^3}$$

$$\frac{n^{r+1}}{n^r}\boxed{P_e} = T^{5/2} e^{-\chi_r/kT} \frac{U^{r+1}(T)}{U^r(T)} \frac{2(2\pi m_e)^{3/2} k^{5/2}}{h^3}$$

Goal: find $\dfrac{n_A^r}{n_A}$

Unknowns:

n^r n^{r+1}

n_e → $P_e = n_e kT$

$\dfrac{n^{r+1}}{n^r}$ is larger when…?

- *T* is large
- The ionization energy χ (from the ground state) is small
- The partition function of the more ionized state U^{r+1} is large
- The partition function of the less ionized state U^r is small
- The partition function of the free election (the free electron "real-estate) is large (i.e. P_e is small)

$$\boxed{\frac{n^{r+1}}{n^r}}\boxed{P_e} = T^{5/2} e^{-\chi_r/kT} \frac{U^{r+1}(T)}{U^r(T)} \frac{2(2\pi m_e)^{3/2} k^{5/2}}{h^3}$$

Relate this "electron pressure" to the total gas pressure

$$P_{\text{total}} = n_{\text{free}} \; kT$$

$$= \frac{(n_{\text{ion}} + n_e)}{n_e} \; kT \, n_e$$

$$= \frac{(n_{\text{ions}} + n_e)}{n_e} \; P_e$$

$$P_e = \frac{n_e / n_{\text{ion}}}{\frac{n_{\text{ion}}}{n_{\text{ion}}} + \frac{n_e}{n_{\text{ion}}}} \; P_{\text{tot}}$$

$$P_e = \frac{E}{1 + E} \; P_{\text{tot}}$$

$$K_r^{r+1}(T,P)$$

$$\frac{n^{r+1}/n_{\text{ion}}}{n^r/n_{\text{ion}}} \frac{E}{1+E} = \boxed{\frac{T^{5/2}}{P_{\text{gas,tot}}} e^{-\chi_r/kT} \frac{U^{r+1}(T,P)}{U^r(T,P)} \frac{2(2\pi m_e)^{3/2} k^{5/2}}{h^3}}$$

Saha for a known P and T

$$K_r^{r+1}(T,P) = \frac{T^{5/2}}{P_{\text{gas,tot}}} e^{-\chi_r/kT} \frac{U^{r+1}(T,P)}{U^r(T,P)} \frac{2(2\pi m_e)^{3/2} k^{5/2}}{h^3}$$

$x^r = \frac{n^r_{\text{ion}}}{n_{\text{ion}}}$ $\qquad U^r(T,P)$: Partition function

$E = \frac{n_e}{n_{\text{ions}}}$ Number of free electron per ion

For each element in the gas mixture:

1 $$\frac{x^{r+1}}{x^r} \frac{E}{1+E} = K_r^{r+1}(T,P)$$

...

2 $$\sum_r x^r = 1$$

Unknowns:

x^r $\quad x^{r+1}$ $\quad \ldots$

E

3 Charge conservation:
How does E relates to all the x^r (of all elements)?

Saha for a known P and T for pure Hydrogen

$$K_r^{r+1}(T,P) = \frac{T^{5/2}}{P_{\text{gas,tot}}} e^{-\chi_r/kT} \frac{U^{r+1}(T,P)}{U^r(T,P)} \frac{2(2\pi m_e)^{3/2} k^{5/2}}{h^3}$$

For each element in the gas mixture:

1. $$\frac{x^{r+1}}{x^r} \frac{E}{1+E} = K_r^{r+1}(T,P)$$ $\Rightarrow$ $$\frac{x_{\mathrm{H}}^{+}}{x_{\mathrm{H}}^{o}} \frac{E}{1+E} = K_o^{+}(T,P)$$

...

2. $$\sum_r x^r = 1$$ $\Rightarrow$ $$x_{\mathrm{H}}^{+} + x_{\mathrm{H}}^{o} = 1$$

3. Charge conservation:
How does E relates to all the x^r (of all elements)? $\Rightarrow$ $$E = x_{\mathrm{H}}^{+}$$

$$E = \frac{n_e}{n_{\text{ions}}}$$

Solve for *E*: $$E = \left(\frac{K_o^{+}}{K_o^{+} + 1} \right)^{1/2}$$

In notebook (Part 1)

- Make a function that returns x_{H^+} for an array of temperature
- Make a graph of x_{H^+} for an array of temperature using your function

A quick parenthesis about the partition function

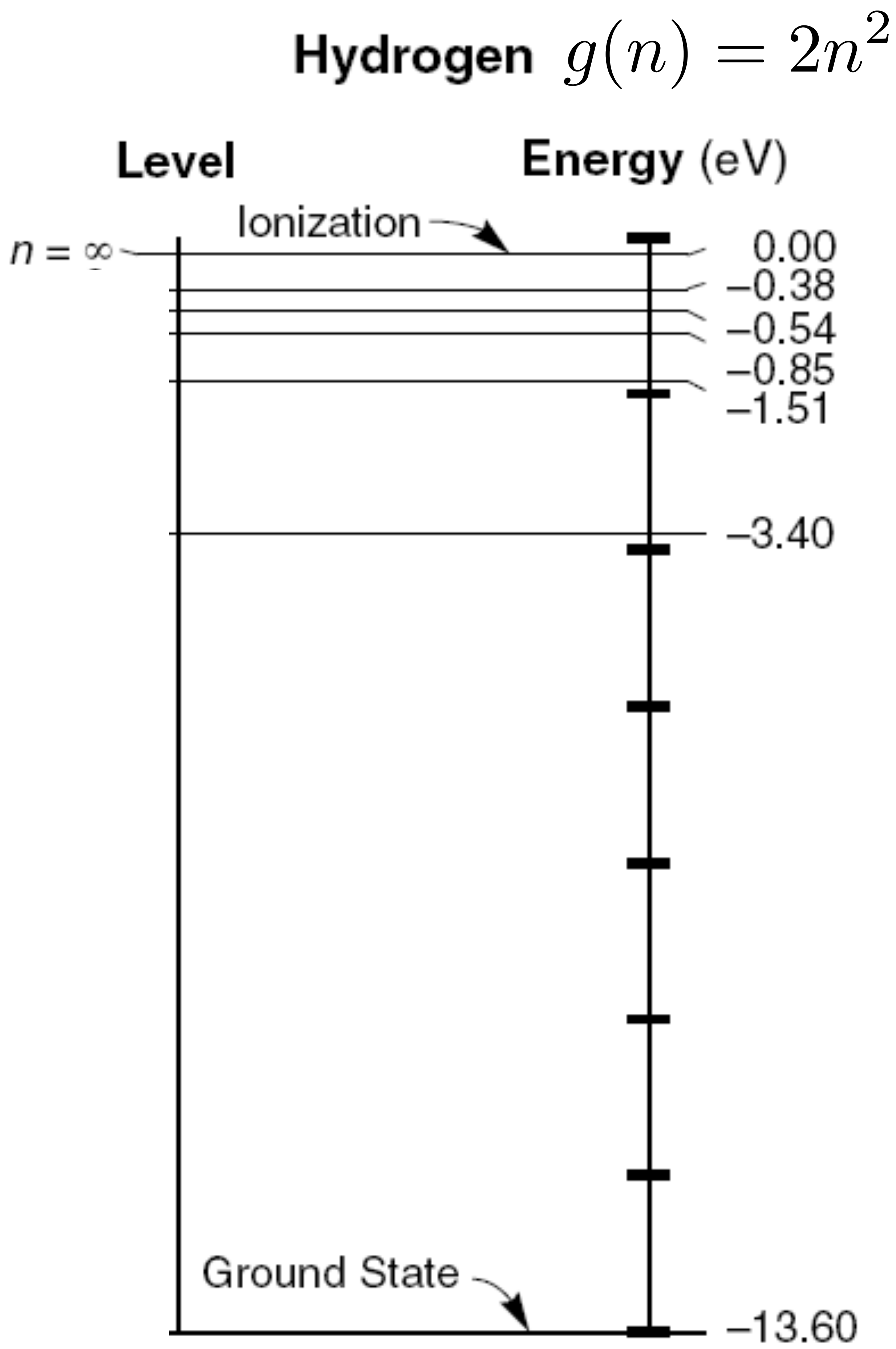
A slide from last week.

For a given ionization state (e.g. H^o):

$$n = \frac{n_o}{g_o} \boxed{\begin{matrix} \sum_s g_s \, e^{-\epsilon_s/kT} \\ \\ U^r(T, s_{max}) \end{matrix}}$$

$$n^r = \frac{n_o^r}{g_o^r}$$

"Partition function"
If we know the structure of the atom,
we can calculate it

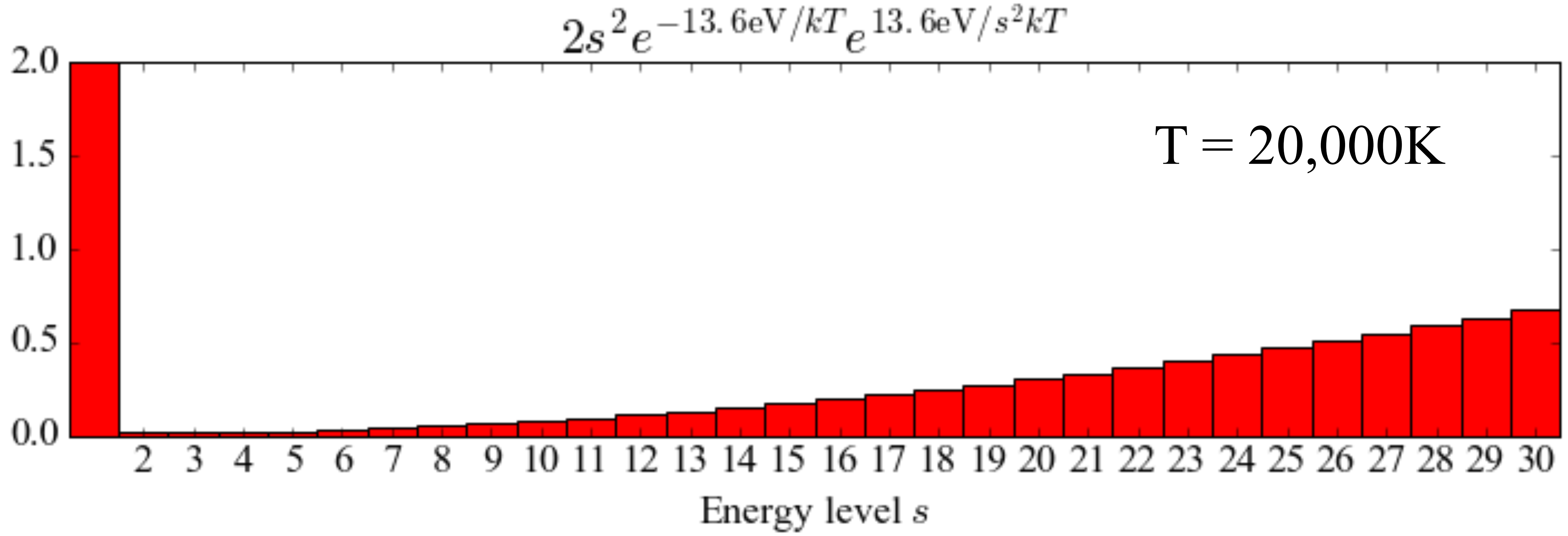


Energy Levels for the Hydrogen Atom

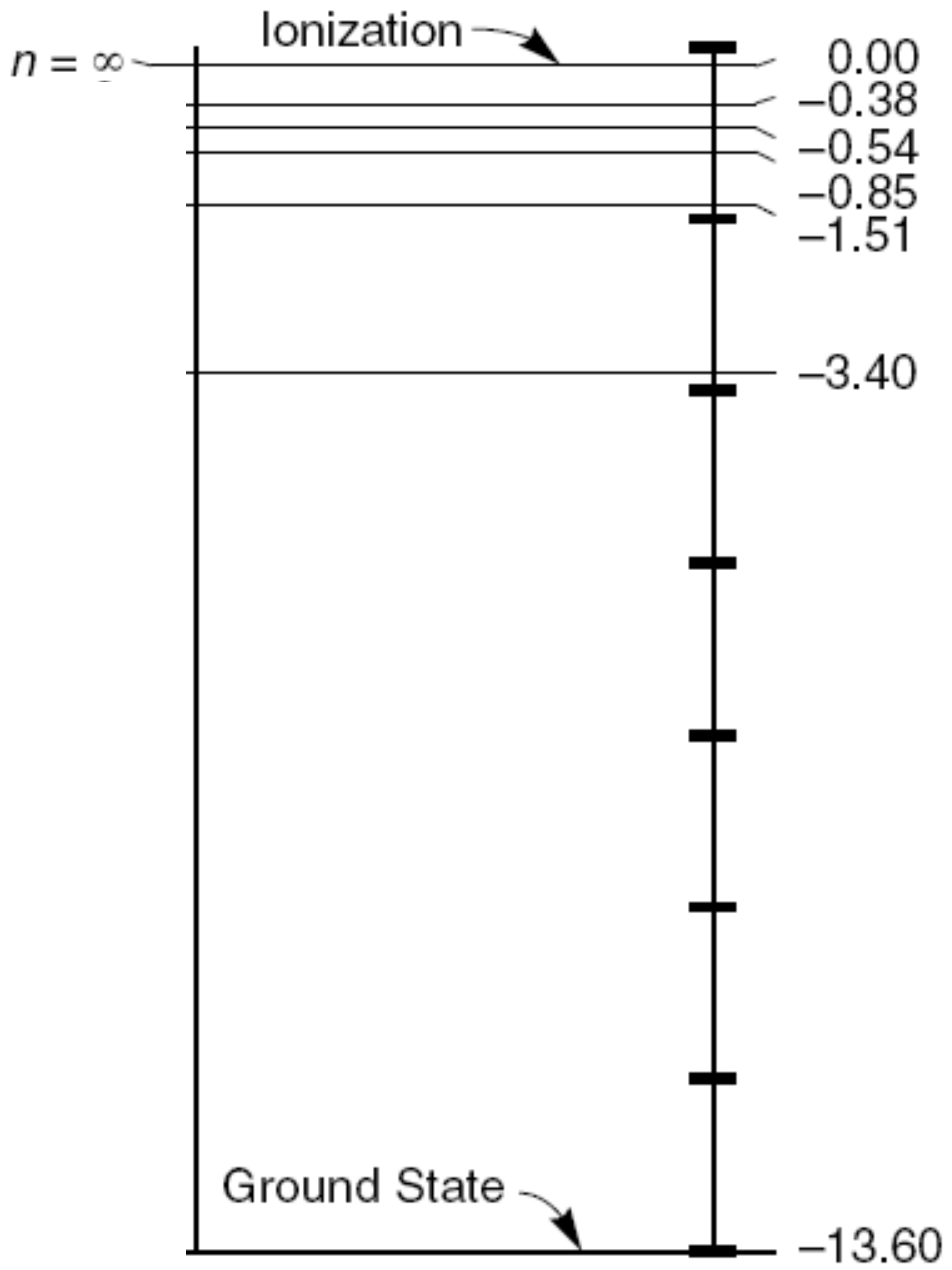
There is a relation between the total population of a given ionization state (e.g H^o) and the population of that ion's ground state (e.g. H^o_o)

$$U^r(T, s_{\max}) = \sum_s g_s\, e^{-\epsilon_s/kT}$$

$$g(n) = 2n^2$$



Hydrogen $g(n) = 2n^2$



Energy Levels for the Hydrogen Atom

If we make the sum over an infinite numbers of energy levels, the partition function would be infinite!

$$\frac{n^{r+1}}{n^r}\boxed{P_e} = T^{5/2} e^{-\chi_r/kT} \frac{U^{r+1}(T)}{U^r(T)} \frac{2(2\pi m_e)^{3/2} k^{5/2}}{h^3}$$

Goal: find $\frac{n_A^r}{n_A}$

Unknowns:

n^r n^{r+1}

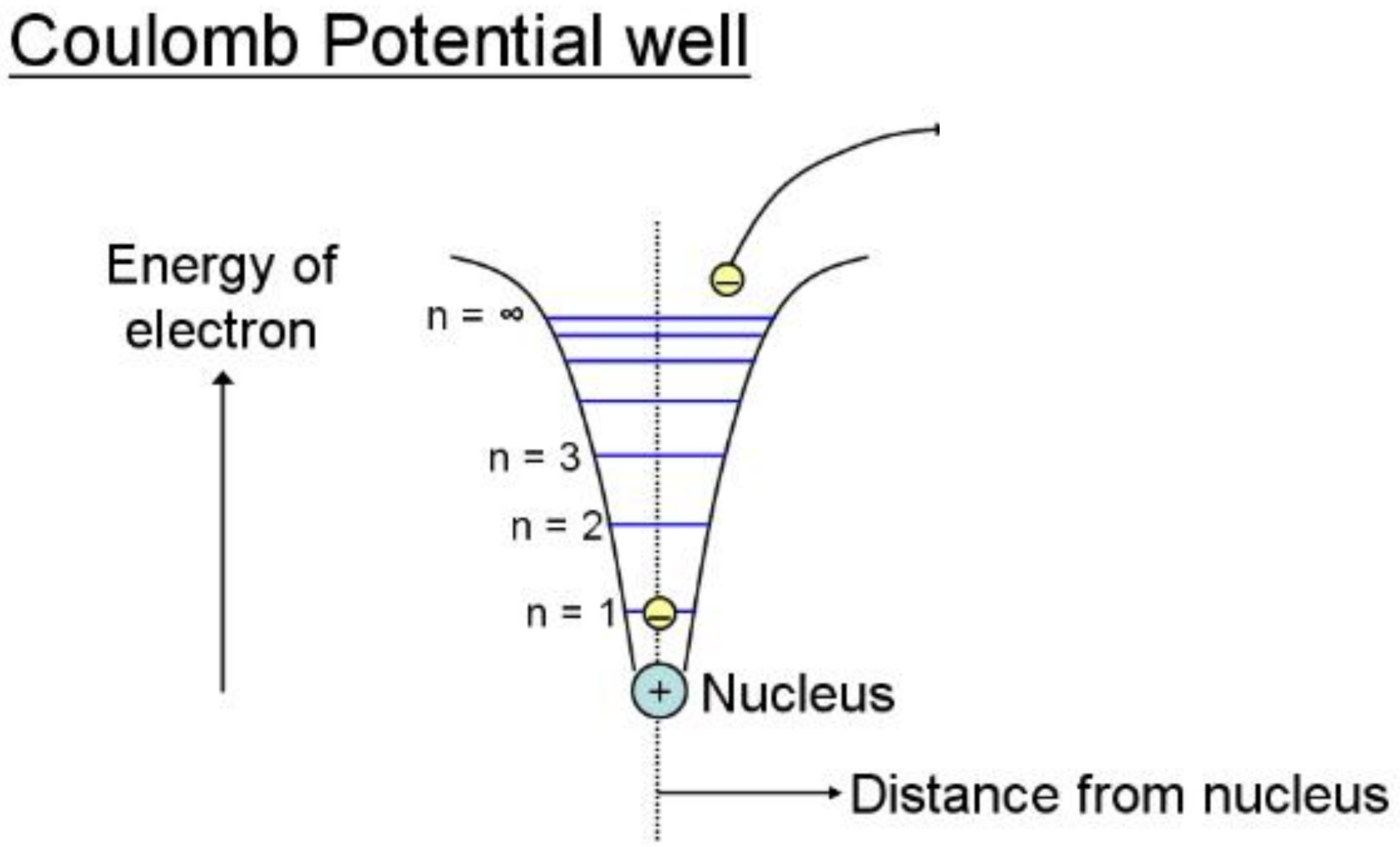
n_e

$P_e = n_e kT$

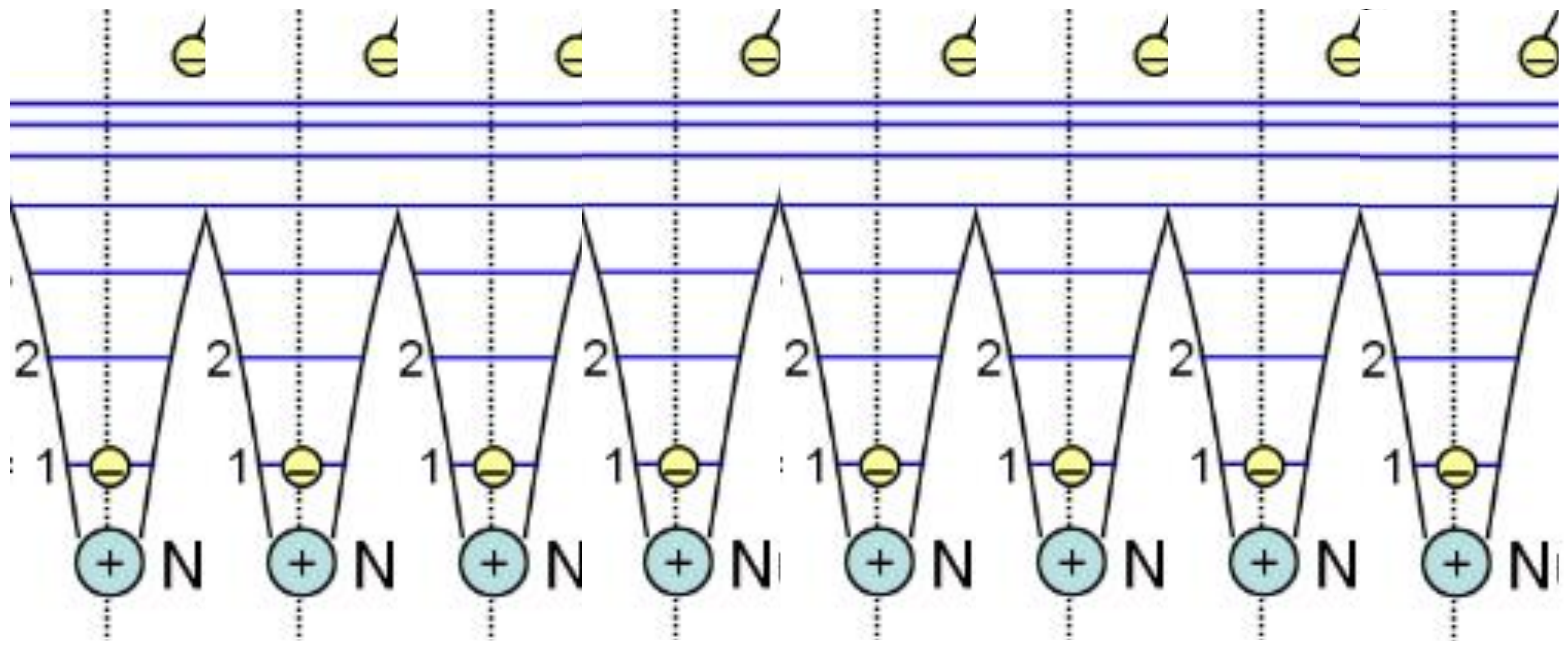
$\frac{n^{r+1}}{n^r}$ is larger when…?

- T is large
- The ionization energy χ (from the ground state) is small
- The partition function of the more ionized state U^{r+1} is large
- **The partition function of the less ionized state U^r is small**
- The partition function of the free election (the free electron "real-estate) is large (i.e. P_e is small)

Idealized case
(a proton alone in the universe

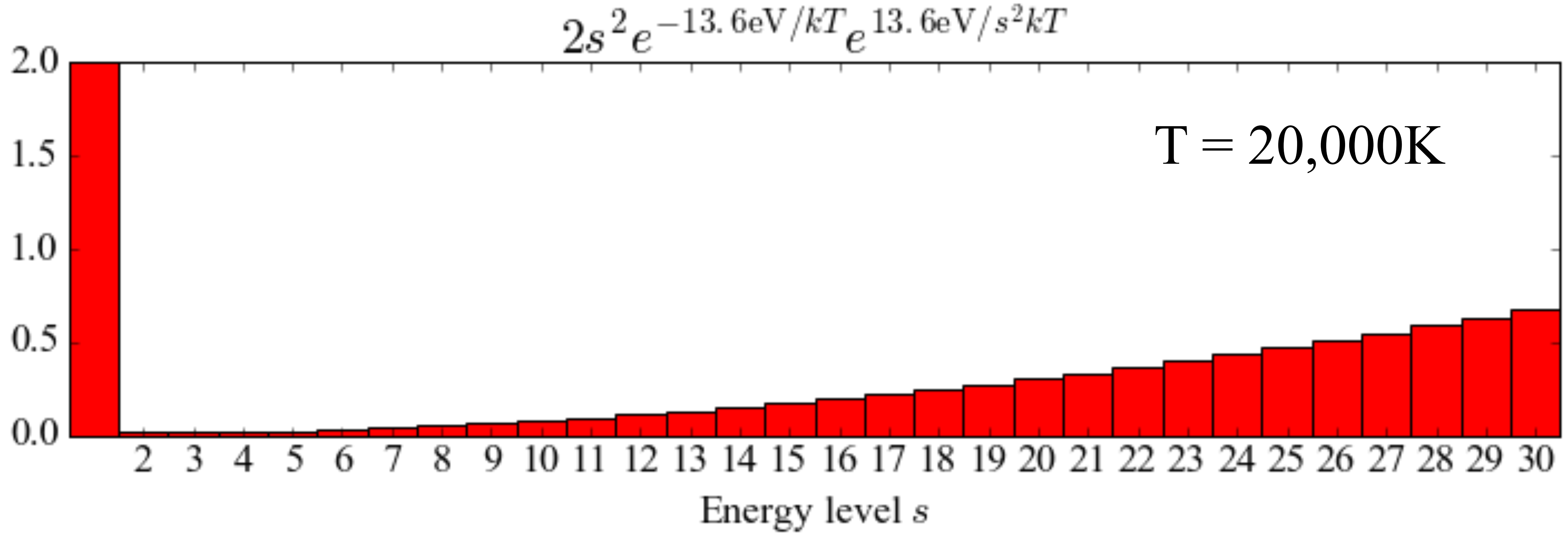


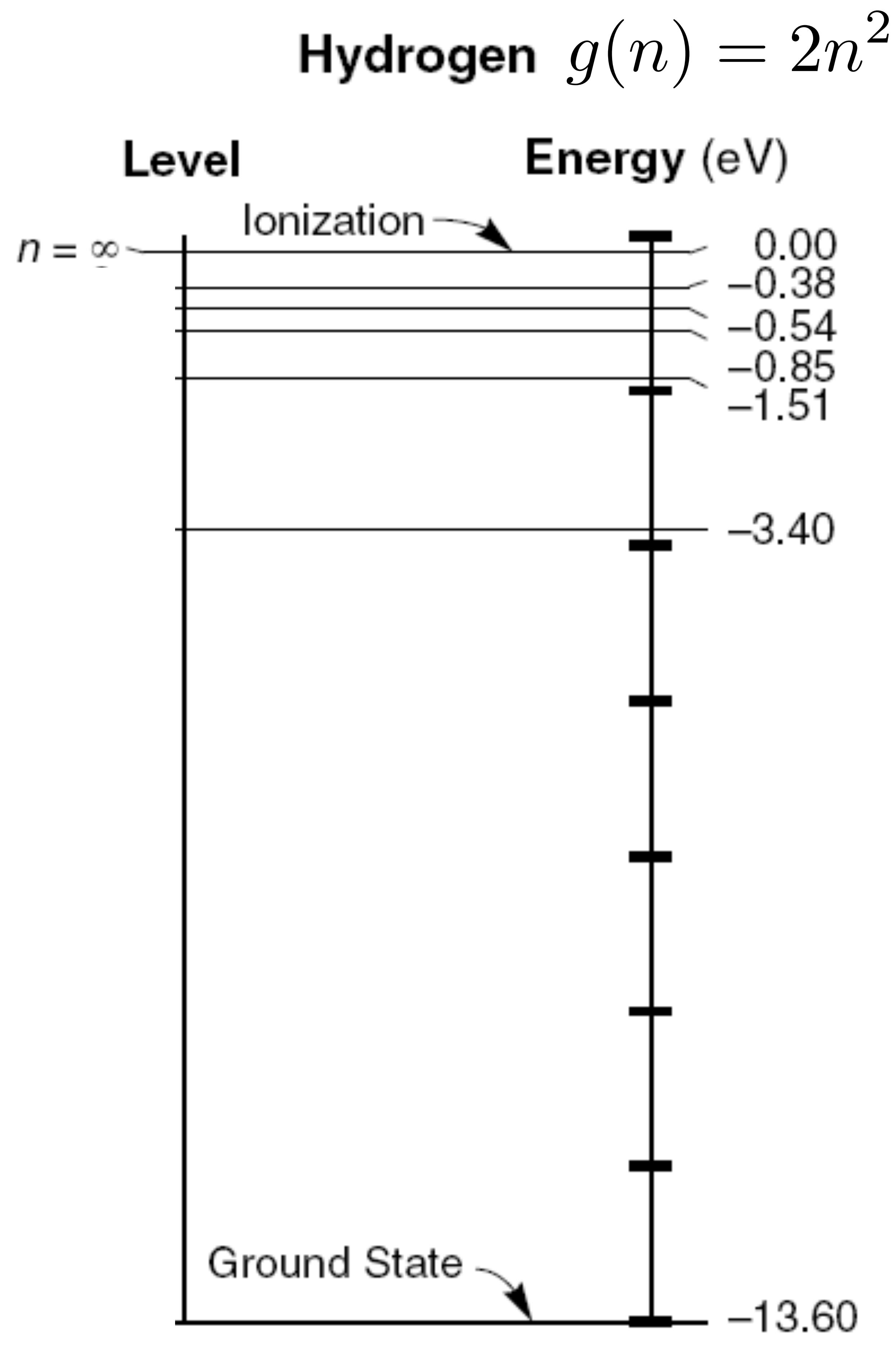
In reality, these upper energy levels don't exists if the density if too high



$$U^r(T, s_{\max}) = \sum_{s}^{s_{\max}} g_s \, e^{-\epsilon_s/kT}$$

$$g(n) = 2n^2$$





Energy Levels for the Hydrogen Atom

If we make the sum over an infinite numbers of energy levels, the partition function would be infinite!

Two factors:

If the pressure is high, the electron getting ionized does not have a lot of free real estate to relocated to.

A

B

Helps ionization

Prevents ionization

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If the pressure is high, the electron getting ionized does not have a lot of free real estate to relocated to.

A Helps ionization

B Prevents ionization

If the pressure is really really high, the lower level atom does not have a lot of upper energy levels.

A Helps ionization

B Prevents ionization

Two factors:

If the pressure is high, the electron getting ionized does not have a lot of free real estate to relocated to.

A

Helps ionization

B

Prevents ionization

If the pressure is really really high, the lower level atom does not have a lot of upper energy levels.

A

Helps ionization

B

Prevents ionization

Saha for a known P and T

$$K_r^{r+1}(T,P) = \frac{T^{5/2}}{P_{\rm gas,tot}} e^{-\chi_r/kT} \frac{U^{r+1}(T,P)}{U^r(T,P)} \frac{2(2\pi m_e)^{3/2} k^{5/2}}{h^3}$$

$$x^r = \frac{n^r_{\rm ion}}{n_{\rm ion}}$$

$U^r(T,P)$: Partition function

$$E = \frac{n_e}{n_{\rm ions}}$$

Number of free electron per ion

For each element in the gas mixture:

1 $$\frac{x^{r+1}}{x^r} \frac{E}{1+E} = K_r^{r+1}(T,P)$$

...

2 $$\sum_r x^r = 1$$

Unknowns:

x^r x^{r+1} ...

E

3 Charge conservation:
How does E relates to all the x^r (of all elements)?

What if we have a mixture of H and He?

$\boxed{E}$ x^o_{H} x^+_{H} x^o_{He} x^+_{He} x^{++}_{He}

Hydrogen

1a
$$\frac{x^+_{\mathrm{H}}}{x^o_{\mathrm{H}}}\frac{\boxed{E}}{1+\boxed{E}} = K^+_{o,\mathrm{H}}(T,P)$$

2a
$$x^o_{\mathrm{H}} + x^+_{\mathrm{H}} = 1$$

Helium

1b
$$\frac{x^+_{\mathrm{He}}}{x^o_{\mathrm{He}}}\frac{\boxed{E}}{1+\boxed{E}} = K^+_{o,\mathrm{He}}(T,P)$$

1c
$$\frac{x^{++}_{\mathrm{He}}}{x^+_{\mathrm{He}}}\frac{\boxed{E}}{1+\boxed{E}} = K^{++}_{+,\mathrm{He}}(T,P)$$

2b
$$x^o_{\mathrm{He}} + x^+_{\mathrm{He}} + x^{++}_{\mathrm{He}} = 1$$

3
$$\boxed{E} = \mu_{\mathrm{ion}}\left[\; X\, x^+_{\mathrm{H}} + \frac{Y}{4}\left(x^+_{\mathrm{He}} + 2x^{++}_{\mathrm{He}}\right) \;\right]$$

$\boxed{E}$ x_{H}^{o} x_{H}^{+} x_{He}^{o} x_{He}^{+} x_{He}^{++}

Hydrogen

1a $$-x_{\mathrm{H}}^{o} K_{o,\mathrm{H}}^{+}(T,P) + x_{\mathrm{H}}^{+}\frac{\boxed{E}}{1+\boxed{E}} = 0$$

2a $$x_{\mathrm{H}}^{o} + x_{\mathrm{H}}^{+} = 1$$

Helium

1b $$-x_{\mathrm{He}}^{o} K_{o,\mathrm{He}}^{+}(T,P) + x_{\mathrm{He}}^{+}\frac{\boxed{E}}{1+\boxed{E}} = 0$$

1c $$-x_{\mathrm{He}}^{+} K_{+,\mathrm{He}}^{++}(T,P) + x_{\mathrm{He}}^{++}\frac{\boxed{E}}{1+\boxed{E}} = 0$$

2b $$x_{\mathrm{He}}^{o} + x_{\mathrm{He}}^{+} + x_{\mathrm{He}}^{++} = 1$$

3 $$\boxed{E} = \mu_{\mathrm{ion}}\left[X x_{\mathrm{H}}^{+} + \frac{Y}{4}\left(x_{\mathrm{He}}^{+} + 2x_{\mathrm{He}}^{++}\right) \right]$$

$\boxed{E}$ x^o_{H} x^+_{H} x^o_{He} x^+_{He} x^{++}_{He}

1a $$-x^o_{\mathrm{H}} K^+_{o,\mathrm{H}}(T,P) + x^+_{\mathrm{H}} \frac{\boxed{E}}{1+\boxed{E}} = 0$$

2a $$x^o_{\mathrm{H}} + x^+_{\mathrm{H}} = 1$$

1b $$-x^o_{\mathrm{He}} K^+_{o,\mathrm{He}}(T,P) + x^+_{\mathrm{He}} \frac{\boxed{E}}{1+\boxed{E}} = 0$$

1c $$-x^+_{\mathrm{He}} K^{++}_{+,\mathrm{He}}(T,P) + x^{++}_{\mathrm{He}} \frac{\boxed{E}}{1+\boxed{E}} = 0$$

2b $$x^o_{\mathrm{He}} + x^+_{\mathrm{He}} + x^{++}_{\mathrm{He}} = 1$$

3 $$\boxed{E} = \mu_{\mathrm{ion}} \left[X x^+_{\mathrm{H}} + \frac{Y}{4}\left(x^+_{\mathrm{He}} + 2x^{++}_{\mathrm{He}}\right) \right]$$

E x_{H}^{o} x_{H}^{+} x_{He}^{o} x_{He}^{+} x_{He}^{++}

1a $$-x_{\mathrm{H}}^{o} K_{o,\mathrm{H}}^{+} + x_{\mathrm{H}}^{+} \frac{E}{1+E} = 0$$

2a $$x_{\mathrm{H}}^{o} + x_{\mathrm{H}}^{+} = 1$$

1b $$-x_{\mathrm{He}}^{o} K_{o,\mathrm{He}}^{+} + x_{\mathrm{He}}^{+} \frac{E}{1+E} = 0$$

1c $$-x_{\mathrm{He}}^{+} K_{+,\mathrm{He}}^{++} + x_{\mathrm{He}}^{++} \frac{E}{1+E} = 0$$

2b $$x_{\mathrm{He}}^{o} + x_{\mathrm{He}}^{+} + x_{\mathrm{He}}^{++} = 1$$

3 $$E = \mu_{\mathrm{ion}} \left[X x_{\mathrm{H}}^{+} + \frac{Y}{4} \left(x_{\mathrm{He}}^{+} + 2 x_{\mathrm{He}}^{++} \right) \right]$$

$\boxed{E}$

$$\begin{array}{c} \text{1a} \\ \text{2a} \\ \text{1b} \\ \text{1c} \\ \text{2b} \end{array}
\begin{bmatrix}
-K^{+}_{o,\mathrm{H}} & \dfrac{\boxed{E}}{1+\boxed{E}} & & & \\
1 & 1 & & & \\
 & & -K^{+}_{o,\mathrm{He}} & \dfrac{\boxed{E}}{1+\boxed{E}} & \\
 & & & -K^{++}_{+,\mathrm{He}} & \dfrac{\boxed{E}}{1+\boxed{E}} \\
 & & 1 & 1 & 1
\end{bmatrix}
\begin{bmatrix} x^{o}_{\mathrm{H}} \\ x^{+}_{\mathrm{H}} \\ x^{o}_{\mathrm{He}} \\ x^{+}_{\mathrm{He}} \\ x^{++}_{\mathrm{He}} \end{bmatrix}
=
\begin{bmatrix} 0 \\ 1 \\ 0 \\ 0 \\ 1 \end{bmatrix}$$

$$\text{3} \quad \boxed{E} = \mu_{\mathrm{ion}} \left[X\, x^{+}_{\mathrm{H}} + \frac{Y}{4}\left(x^{+}_{\mathrm{He}} + 2 x^{++}_{\mathrm{He}} \right) \right]$$

$\boxed{E}$ = guess (step 1)

$$
\begin{array}{c}
\text{1a} \\[2em] \text{2a} \\[2em] \text{1b} \\[2em] \text{1c} \\[2em] \text{2b}
\end{array}
\begin{bmatrix}
-K^{+}_{o,\mathrm{H}} & \dfrac{\boxed{E}}{1+\boxed{E}} & & & \\
1 & 1 & & & \\
 & & -K^{+}_{o,\mathrm{He}} & \dfrac{\boxed{E}}{1+\boxed{E}} & \\
 & & & -K^{++}_{+,\mathrm{He}} & \dfrac{\boxed{E}}{1+\boxed{E}} \\
 & & 1 & 1 & 1
\end{bmatrix}
\begin{bmatrix}
x^{o}_{\mathrm{H}} \\ x^{+}_{\mathrm{H}} \\ x^{o}_{\mathrm{He}} \\ x^{+}_{\mathrm{He}} \\ x^{++}_{\mathrm{He}}
\end{bmatrix}
=
\begin{bmatrix}
0 \\ 1 \\ 0 \\ 0 \\ 1
\end{bmatrix}
$$

3 $$\boxed{E} = \mu_{\mathrm{ion}} \left[X x^{+}_{\mathrm{H}} + \frac{Y}{4} \left(x^{+}_{\mathrm{He}} + 2 x^{++}_{\mathrm{He}} \right) \right]$$

$\boxed{E}$ = guess (step 1)

Step 5: Does it match your guess? No.. → **Keep guessing..**

Yes! → **That's the solution!**

Step 2: Calculate this matrix

Step 3: Solve for these

$$
\begin{array}{c}
1a \\ 2a \\ 1b \\ 1c \\ 2b
\end{array}
\begin{bmatrix}
-K^{+}_{o,\mathrm{H}} & \dfrac{\boxed{E}}{1+\boxed{E}} & & & \\
1 & 1 & & & \\
 & & -K^{+}_{o,\mathrm{He}} & \dfrac{\boxed{E}}{1+\boxed{E}} & \\
 & & & -K^{++}_{+,\mathrm{He}} & \dfrac{\boxed{E}}{1+\boxed{E}} \\
 & & 1 & 1 & 1
\end{bmatrix}
\begin{bmatrix}
x^{o}_{\mathrm{H}} \\ x^{+}_{\mathrm{H}} \\ x^{o}_{\mathrm{He}} \\ x^{+}_{\mathrm{He}} \\ x^{++}_{\mathrm{He}}
\end{bmatrix}
=
\begin{bmatrix}
0 \\ 1 \\ 0 \\ 0 \\ 1
\end{bmatrix}
$$

Step 4: Calculate E

$$
3 \qquad \boxed{E} = \mu_{\mathrm{ion}} \left[X x^{+}_{\mathrm{H}} + \frac{Y}{4}\left(x^{+}_{\mathrm{He}} + 2x^{++}_{\mathrm{He}}\right) \right]
$$

In your notebook:

- Demo of this procedure
- Mini-project at home (for a “A” on the notebook)